Overview of OpenSRS

TOWARD AN OPEN IMPLEMENTATION OF ISO 11238

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NCATS

NIH National Center for Advancing Translational Sciences

The proposed implementation is a cultivation of our efforts over the years to *develop*, *demonstrate*, and *disseminate* software for managing, mining, and visualizing chemical biology data.

Outline

- ISO 11238 and scope
- Reference substance database
- Software requirements
- Implementation roadmap
- Architecture overview
- Technology stack
- Status & milestones
- Discussion (and demo)

ISO 11238 and Scope

- Substance categories
  - Chemical
  - Protein
  - Nucleic acid
  - Polymer
  - Structurally diverse
- Specified substances Groups 1–4
- Official names in multiple languages, jurisdictions, and domains
- Well-defined references and relationships between substances
- Unique identifiers

Reference Substance Database

- A reference substance database is distributed with each OpenSRS deployment
  - » Bootstrap from FDA's public SRS records
- A public accessible "master" copy of the database is housed at NCATS
  - » Data curation
  - » Conflict resolution
- Defined update schedule

Software Requirements

- Self-contained and modular
  - » Run entirely on a desktop or access remotely
- Well-defined data access application programming interface (API)
  - » Mobile or third-party clients
- Fine-gained security model
  - » Access control for every piece of information
- Audit trail of all data fields
- Web- and desktop-based clients
  - » Multiple platforms (e.g., Linux, Windows, Mac) for desktop client
- Basic support for text, structure, sequence searching
- Wizard interface to guide registration
- Support attachments (e.g., PDF's, MS spectra, images)
- Configurable "business rules" for standardizing structures

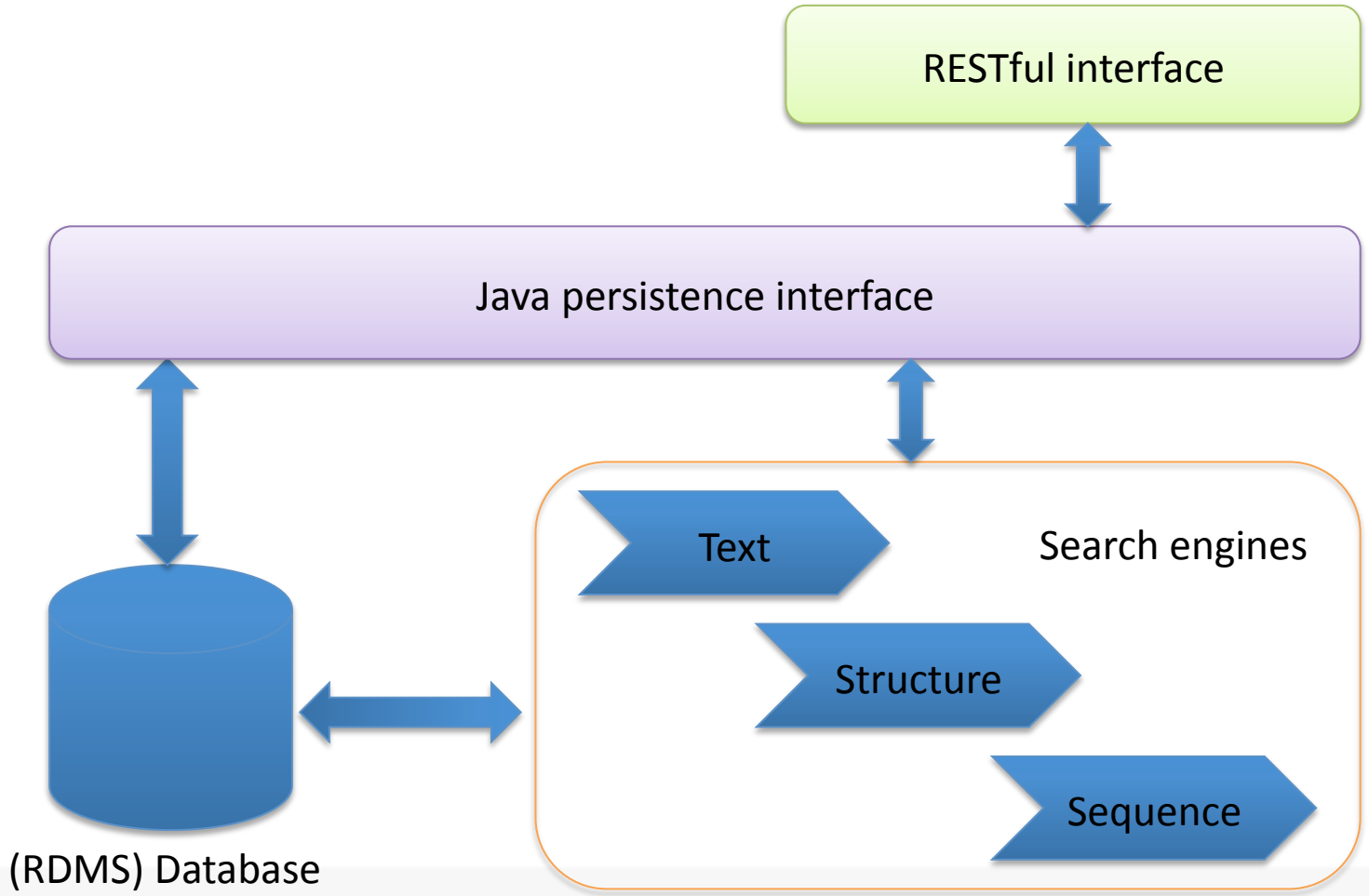
Implementation Roadmap

- Multiple stages
- Stage I (alpha)
  - » Use cases limited to FDA & CBG-MEB
  - » Solidify backend and data models
  - » Chemical substance
- Stage II (beta)
  - » Limited deployment at FDA
  - » Support polymer & protein substances
- Stage III (beta)
  - » Support for remaining substance categories
  - » ISO 11238 compliance
  - » Open deployments to other organizations
- Stage IV (public release)

Architecture Overview

- Client-server
  - » Server is self-hosting when installed on desktop
- Backend database agnostic (e.g., Oracle, MySQL)
- Support two APIs: Native (Java) and RESTful
- Standalone server or deployable within a standard web container (e.g., Glassfish, Tomcat)
- Pluggable chemical toolkit
  - » Default toolkit is a redistributable version of JChem
- Pluggable engines for text, structure, and sequence searching

Architecture Overview (cont'd)



Technology Stack

- Web-based client
  - » Combination of client- and server-side technologies (e.g., ExtJS, JSF)
- Desktop client
  - » Java Swing and other open source libraries
  - » Deploy as either signed webstart or installed image
- Server
  - » JDO as the persistence layer
  - » Lucene text search engine
  - » Custom implementations of structure and sequence search engines
  - » Standalone server based on embedded Jetty or Glassfish and H2 database

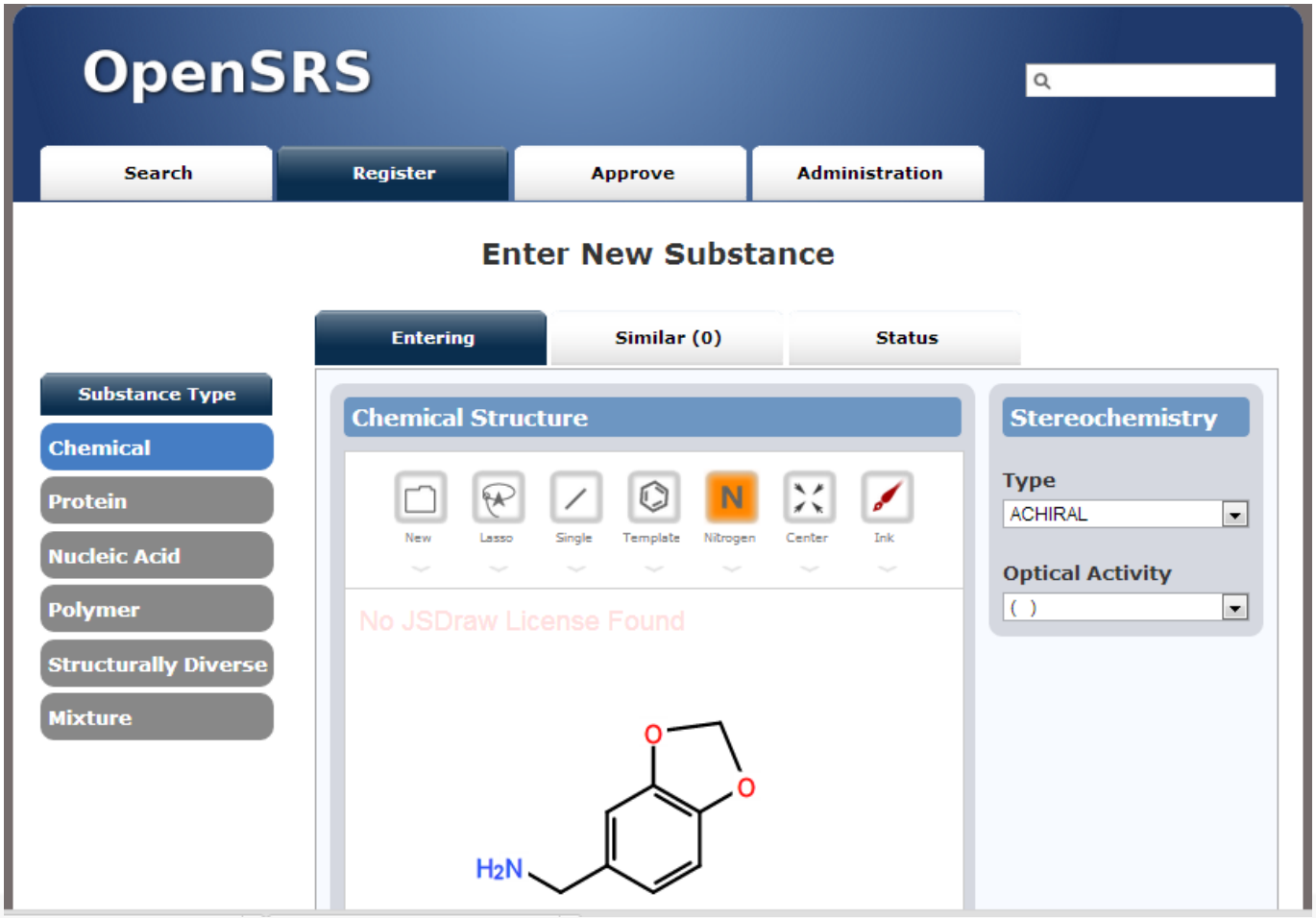
Status & Milestones

- Basic user interface framework for web and desktop clients in place
- On-going development on the server backend
  - » Solidify the Java persistence API
  - » Develop initial set of “business rules”
  - » RESTful API
- Anticipate completion of Stage I in June 2013
- If all goes well, Stage II by early 2014

Discussion

- Organic development model
  - » Features evolve through iterations
- Code is hosted at bitbucket.org
  - » Repository is currently private but access is available upon request
  - » Repository goes public in Stage II (beta)
- Demos available for web and desktop clients

Web Client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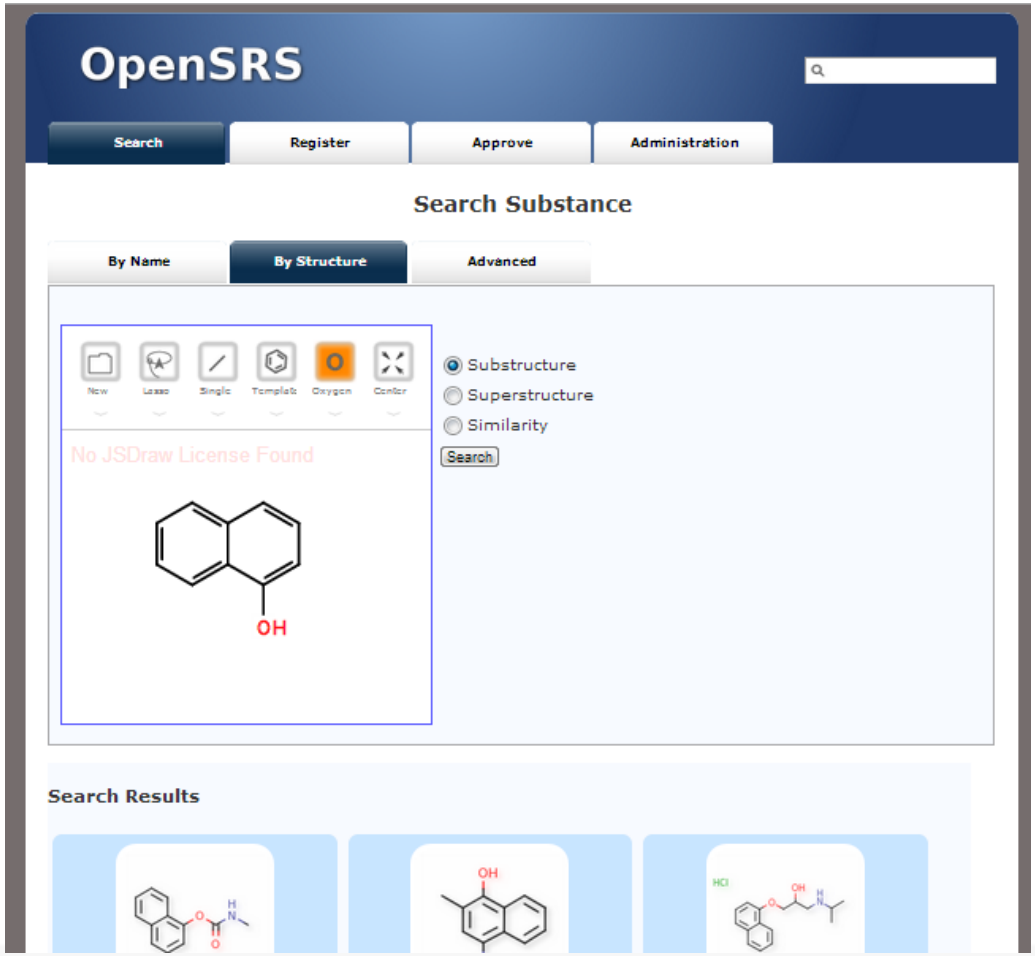
Web Client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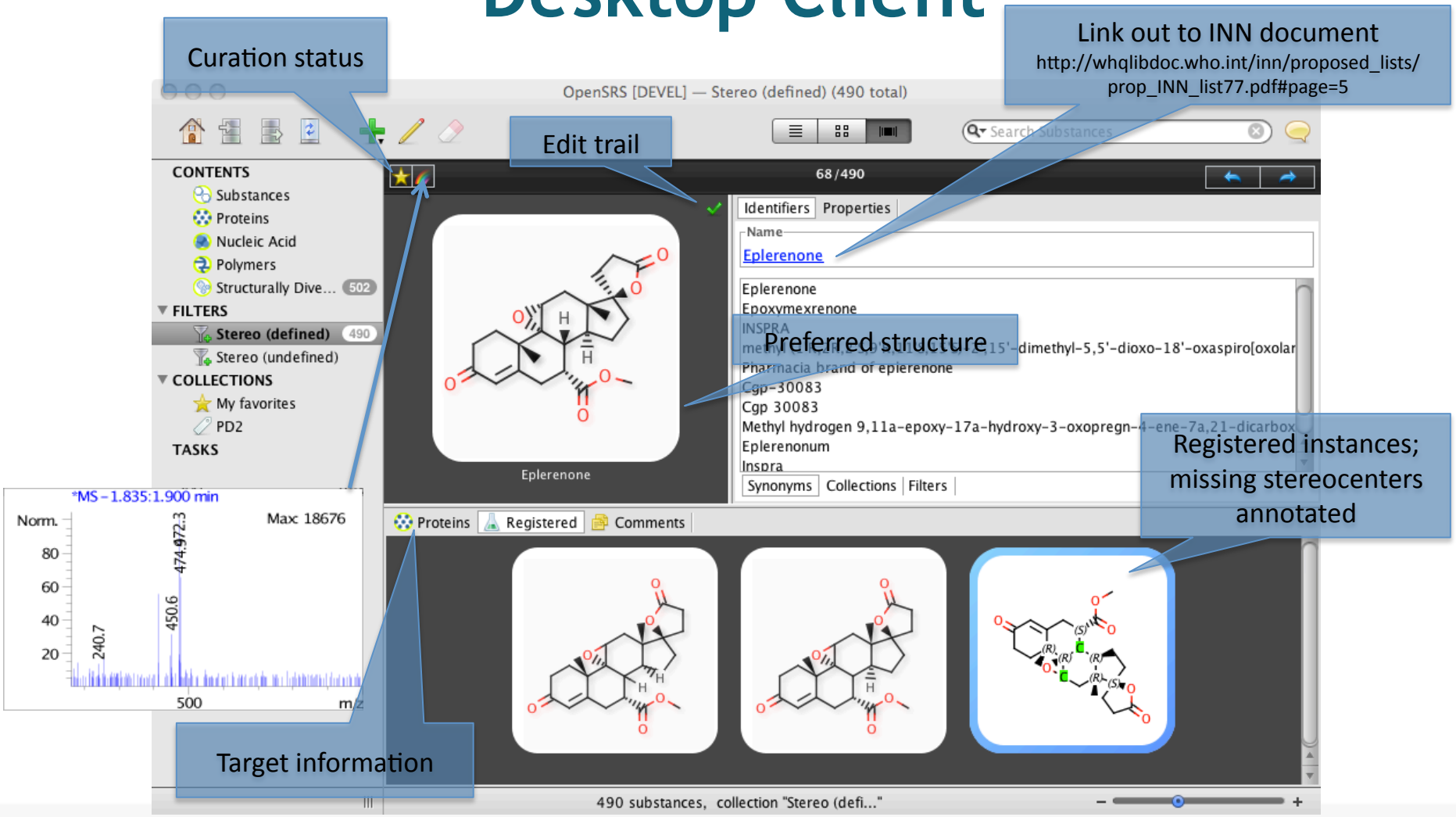
Desktop Client



Desktop Client